

Toroidal moments of Schrödinger eigenstates

M. Encinosa^{a,*}, J. Williamson^a

^a*Florida A&M University, Department of Physics, Tallahassee FL, 32307*

Abstract

The Hamiltonian for a particle constrained to motion near a toroidal helix with loops of arbitrary eccentricity is developed. The resulting three dimensional Schrödinger equation is reduced to a one dimensional effective equation inclusive of curvature effects. A basis set is employed to find low-lying eigenfunctions of the helix. Toroidal moments corresponding to the individual eigenfunctions are calculated. The dependence of the toroidal moments on the eccentricity of the loops is reported. Unlike the classical case, the moments strongly depend on the details of loop eccentricity.

Keywords: toroidal helix, toroidal moment, curvature potential

1. Introduction

The majority of work directed towards modeling the metaparticle constituents of metamaterials has been performed using classical physics [1]. The characteristic length scales of most currently fabricated metaparticles allow for that approach to be appropriate and productive. However, it is nearly certain that metaparticles will eventually be fabricated on scales at which quantum mechanical methods will prove necessary to capture their physics with good fidelity [2, 3, 4].

This paper focuses upon two interesting properties common to many metaparticles: they can be approximated as reduced dimensionality systems and they

*Corresponding Author

Email addresses: mario.encinosa@fam.u.edu (M. Encinosa),
johnny.williamson@cepast.fam.u.edu (J. Williamson)

can possess nontrivial topologies. The advent of quasi one and two dimensional curved nanostructures has led to situations wherein formalism developed for particles constrained to curved manifolds has become of practical importance. Specifically, there exists a prescription that allows for degrees of freedom extraneous to the particle's 'motion' on a curve or surface to be shuttled into effective curvature potentials in the Schrödinger equation [5, 6, 7, 8, 9, 10, 11, 12, 13, 14].

Recently, it was suggested that quantum methods be employed in an effort towards understanding toroidal moments induced by currents supported on nanoscale metaparticles and the interactions of those moments with time-dependent electromagnetic fields [15]. Because of the theoretical and practical interest in toroidal moments [16, 17, 18, 19, 20, 21, 22], a toroidal helix (TH) of adjustable eccentricity has been chosen here to investigate the role of quantum effects. Being closed, a TH can support current carrying solutions allowing for the existence of a toroidal moment [23]. Furthermore, the TH has the advantage of having sufficient symmetry to allow for a clean reduction of the full Hamiltonian to a one dimensional effective Hamiltonian.

The goals of this work are threefold. The first is to derive the Hamiltonian for a particle in a coordinate system adapted to include points near the coils of a TH of arbitrary eccentricity. The next deals with reducing the full three dimensional Hamiltonian via a well known procedure [6, 24, 25] to arrive at an effective one-dimensional Schrödinger equation. The reduction of dimensionality impels the introduction of a curvature potential well known to workers in the field of curved manifold quantum mechanics. A basis set consistent with the periodicity and symmetry of the system is introduced thereafter. Achieving the first two goals and with the basis functions in hand, the spectrum and wave functions of the system (which can be used for applications in the external field and/or time-dependent case) are found. Finally, toroidal moments corresponding to particular eigenstates are determined and their sensitivity to the eccentricity of the loops comprising the TH is investigated.

The remainder of this paper is organized into four sections. Section 2 introduces a parameterization for an ω turn TH in terms of an azimuthal coordinate

ϕ . A three dimensional Hamiltonian H_ω^3 appropriate to motion near the TH follows by attaching a Frenet system to the helix and assigning two coordinates q_N, q_B to describe degrees of freedom away from the coil. Section 3 details the reduction of H_ω^3 to a one-dimensional H_ω^1 by standard methods, although perhaps unfamiliar to workers in the metamaterial community. As a consequence of the reduction, curvature potentials appear. Their presence has been shown to be essential in properly describing one dimensional systems that exist in an ambient higher dimensional space [26]. Section 4 presents the basis set used to calculate the spectrum, eigenstates and toroidal moments per a given quantum state. Those quantities, along with results showing the dependence of TMs on eccentricity are given. Section 5 is dedicated to conclusions and some remarks concerning future work.

2. The TH Schrödinger equation

To arrive at the time independent Schrödinger equation $H_\omega^3(\mathbf{r})\Psi = E\Psi = (-\frac{1}{2}\nabla^2 + V)\Psi$, the Laplacian must be derived from a suitable parameterization of the TH geometry. Consider a TH with ω equally spaced circular coils. Let R be the distance from the z-axis to a loop center and a the radius of a loop. First define

$$W(\phi) = R + a \cos(\omega\phi) \quad (1)$$

with ϕ the usual cylindrical coordinate azimuthal angle. The circular TH is traced out by the Monge form [27]

$$\mathbf{r}(\phi) = W(\phi)\hat{\rho} + a \sin(\omega\phi)\hat{\mathbf{k}}. \quad (2)$$

Generalizing Eq.(2) to coils of arbitrary eccentricity requires only the modification

$$\mathbf{r}(\phi) = W(\phi)\hat{\rho} + b \sin(\omega\phi)\hat{\mathbf{k}} \quad (3)$$

where a, b may be adjusted to yield the coil shape desired (Fig. 1). To avoid cluttering the narrative with blocks of equations, the expressions that follow

will apply to the circular case only. The expressions for arbitrary a and b are given in the appendix.

A three dimensional neighborhood in the vicinity of the TH is built by assigning two coordinates to points near the curve along unit vectors orthogonal to the curve's tangent and to each other. The Frenet-Serret equations [27] provide such an orthonormal coordinate system known as a Frenet trihedron. The unit tangent to any point on a curve traced by $\mathbf{r}(\phi)$ is

$$\hat{\mathbf{T}} = \frac{d\mathbf{r}(\phi)}{d\phi} \left\| \frac{d\mathbf{r}(\phi)}{d\phi} \right\|^{-1} \quad (4)$$

from which the Frenet trihedron can be constructed via the relations

$$\frac{d\hat{\mathbf{T}}}{d\phi} = \left\| \frac{d\mathbf{r}(\phi)}{d\phi} \right\| \kappa(\phi) \hat{\mathbf{N}} \quad (5)$$

$$\frac{d\hat{\mathbf{N}}}{d\phi} = \left\| \frac{d\mathbf{r}(\phi)}{d\phi} \right\| (-\kappa(\phi) \hat{\mathbf{T}} + \tau(\phi) \hat{\mathbf{B}}) \quad (6)$$

$$\frac{d\hat{\mathbf{B}}}{d\phi} = -\left\| \frac{d\mathbf{r}(\phi)}{d\phi} \right\| \tau(\phi) \hat{\mathbf{N}} \quad (7)$$

where the curvature and torsion of the space curve $\mathbf{r}(\phi)$ are indicated by $\kappa(\phi)$ and $\tau(\phi)$ respectively (where again, detailed forms for the expressions in Eqs. (4-7) appear in the appendix). Points near the TH are located via two perpendicular displacements $q_N \hat{\mathbf{N}}$ and $q_B \hat{\mathbf{B}}$. The TH position vector may now be written

$$\mathbf{x}(\phi, q_N, q_B) = \mathbf{r}(\phi) + q_N \hat{\mathbf{N}} + q_B \hat{\mathbf{B}}. \quad (8)$$

It should be noted that Eq.(8) defines a Cartesian region about a curve traced by $\mathbf{r}(\phi)$. While it is certainly possible to construct a finite tubular neighborhood about $\mathbf{r}(\phi)$, the coordinate ambiguity of the azimuthal angle as the radial distance approaches zero causes the limiting procedure to become complicated. Additionally, the separability of the Schrödinger equation into tangential and normal variables is lost, and with it any real advantage in using the reduced Hamiltonian.

The covariant metric tensor elements g_{ij} can be read off of the quadratic form [28]

$$d\mathbf{x} \cdot d\mathbf{x} = g_{ij} dq^i dq^j \quad (9)$$

where in what follows the ordering convention is $(q^1, q^2, q^3) \equiv (\phi, q_N, q_B)$. The Laplacian is

$$\nabla^2 = \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^i} \left(\sqrt{g} g^{ij} \frac{\partial}{\partial q^j} \right) \quad (10)$$

with $g = \det(g_{ij})$ and g^{ij} the contravariant components of the metric tensor.

Before presenting explicit forms for g_{ij} and g^{ij} , it is useful to define

$$f(\phi) = \left\| \frac{d\mathbf{r}(\phi)}{d\phi} \right\| = [(a\omega)^2 + W(\phi)^2]^{1/2} \quad (11)$$

and

$$G(\phi, q_N) = 1 - q_N \kappa(\phi) \quad (12)$$

after which the covariant metric may be written

$$g_{ij} = \begin{pmatrix} f(\phi)^2 [G(\phi, q_N)^2 + \tau(\phi)^2 (q_N^2 + q_B^2)] & -\tau(\phi) q_B f(\phi) & \tau(\phi) q_N f(\phi) \\ -\tau(\phi) q_B f(\phi) & 1 & 0 \\ \tau(\phi) q_N f(\phi) & 0 & 1 \end{pmatrix}. \quad (13)$$

The contravariant form of the metric is obtained straightforwardly;

$$g^{ij} = \frac{1}{f(\phi)^2 G(\phi, q_N)^2} \begin{pmatrix} 1 & \tau(\phi) q_B f(\phi) & -\tau(\phi) q_N f(\phi) \\ \tau(\phi) q_B f(\phi) & f(\phi)^2 [G(\phi, q_N)^2 + \tau(\phi)^2 q_B^2] & -\tau(\phi)^2 q_N q_B f(\phi)^2 \\ -\tau(\phi) q_N f(\phi) & -\tau(\phi)^2 q_N q_B f(\phi)^2 & f(\phi)^2 [G(\phi, q_N)^2 + \tau(\phi)^2 q_N^2] \end{pmatrix}. \quad (14)$$

It is easy to show that

$$\sqrt{g} = f(\phi) (1 - q_N \kappa(\phi)).$$

The Laplacian found by directly evaluating Eq.(10) is complicated by the existence of cross terms arising from $\partial^2 / \partial q^i \partial q^j$, ($i \neq j$), operations. However, all of those terms are multiplied by the distance parameters q_N and q_B such that in the limit $q_N, q_B \rightarrow 0$ they vanish independently of the derivative operators that follow them. Taking this limit now (it will be taken again later post operation

of the $q_{N,B}$ derivatives) leads to a more convenient starting point for developing the reduced Hamiltonian in the ensuing section. Physically, the limiting procedure is effected by external mechanical or electrical constraints; mathematically, they are added by hand into the Schrödinger equation as potentials $V_n(q)$ normal to the lower dimensionality base manifold. Their detailed forms are not important. Previous work has shown that even for finite thicknesses, degrees of freedom extraneous to those of the base manifold do not mix with the latter in the sense that their wave functions decouple [26]. Here, for the sake of definiteness, hard wall potentials are assumed for $V_n(q_N)$ and $V_n(q_B)$ in this and the next section. With this discussion in mind, H_ω^3 may be written as (with $\hbar = m = 1$)

$$H_\omega^3 = -\frac{1}{2} \left(\frac{1}{f(\phi)^2} \frac{\partial^2}{\partial \phi^2} - \frac{f'(\phi)}{f(\phi)^3} \frac{\partial}{\partial \phi} - \kappa(\phi) \frac{\partial}{\partial q_N} + \frac{\partial^2}{\partial q_N^2} + \frac{\partial^2}{\partial q_B^2} \right) + V_n(q_N) + V_n(q_B). \quad (15)$$

Note that the H_ω^3 at this stage is still not separable. The procedure for rendering H_ω^3 separable and arriving at a simpler effective Hamiltonian is given in the following section.

3. Constructing the effective Hamiltonian

As the particle is constrained to the toroidal helix, its wave function will decouple into tangent and normal functions (the subscripts t and n denote tangent and normal respectively)

$$\Psi(\phi, q_N, q_B) \rightarrow \chi_t(\phi) \chi_n(q_N) \chi_n(q_B) \quad (16)$$

and $G(\phi, q_N)$ will approach unity. The normalization condition

$$\int_0^{2\pi} |\Psi(\phi, q_N, q_B)|^2 G(\phi, q_N) f(\phi) d\phi dq_N dq_B = 1 \quad (17)$$

becomes

$$\int_0^{2\pi} |\chi_t(\phi)|^2 |\chi_n(q_N)|^2 |\chi_n(q_B)|^2 f(\phi) d\phi dq_N dq_B = 1. \quad (18)$$

The norm must be conserved in the decoupled limit [6], which implies

$$|\Psi(\phi, q_N, q_B)|^2 G(\phi, q_N) = |\chi_t(\phi)|^2 |\chi_n(q_N)|^2 |\chi_n(q_B)|^2. \quad (19)$$

The wave function $\Psi(\phi, q_N, q_B)$ is now related to $\chi_t(\phi)\chi_n(q_N)\chi_n(q_B)$ by

$$\Psi(\phi, q_N, q_B) = \chi_t(\phi)\chi_n(q_N)\chi_n(q_B)G^{-1/2}(\phi, q_N). \quad (20)$$

Applying H_ω^3 to $\Psi(\phi, q_N, q_B)$ and taking the limit as $q_N, q_B \rightarrow 0$ post all derivative operations yields the result

$$H_\omega^3 = -\frac{1}{2} \left(\frac{1}{f(\phi)^2} \frac{\partial^2}{\partial \phi^2} - \frac{f'(\phi)}{f(\phi)^3} \frac{\partial}{\partial \phi} + \frac{1}{4} \kappa^2(\phi) + \frac{\partial^2}{\partial q_N^2} + \frac{\partial^2}{\partial q_B^2} \right) + V_n(q_N) + V_n(q_B). \quad (21)$$

Distributing the energy between the (ϕ, q_N, q_B) degrees of freedom by allowing $E = E_\phi + E_N + E_B$, leads to the decoupled system

$$-\frac{1}{2} \left(\frac{1}{f(\phi)^2} \frac{\partial^2}{\partial \phi^2} - \frac{f'(\phi)}{f(\phi)^3} \frac{\partial}{\partial \phi} + \frac{1}{4} \kappa^2(\phi) \right) \chi_t(\phi) = E_\phi \chi_t(\phi) \quad (22)$$

$$-\frac{1}{2} \frac{\partial^2 \chi_n(q_N)}{\partial q_N^2} + V_n(q_N) \chi_n(q_N) = E_N \chi_n(q_N) \quad (23)$$

$$-\frac{1}{2} \frac{\partial^2 \chi_n(q_B)}{\partial q_B^2} + V_n(q_B) \chi_n(q_B) = E_B \chi_n(q_B). \quad (24)$$

Since $V(q_N)$ and $V(q_B)$ are the confining potentials effecting the $q_N, q_B \rightarrow 0$ constraint, q_N and q_B can be considered spectator variables and only the ϕ -dependent part of the Hamiltonian indicated in Eq.(21) is nontrivial. The Hamiltonian in one dimension H_ω^1 is written

$$H_\omega^1 = -\frac{1}{2} \left(\frac{1}{f(\phi)^2} \frac{\partial^2}{\partial \phi^2} - \frac{f'(\phi)}{f(\phi)^3} \frac{\partial}{\partial \phi} \right) + V_c(\phi) \quad (25)$$

with

$$V_c(\phi) = -\frac{1}{8} \kappa^2(\phi) \quad (26)$$

the curvature potential. The curvature potential $V_c(\phi)$ emerges as an artifact of embedding the particle's one dimensional path of motion in the ambient three dimensional space. The explicit form of the curvature potential in Eq.(26) can be determined from

$$\kappa(\phi) = [P_1(\phi)^2 + P_2(\phi)^2]^{1/2} \quad (27)$$

where

$$P_1(\phi) = -\frac{a\omega^2 + W(\phi)\cos(\omega\phi)}{f(\phi)^2} \quad (28)$$

and

$$P_2(\phi) = \frac{\sin(\omega\phi)}{f(\phi)} \left[1 + \left(\frac{a\omega}{f(\phi)} \right)^2 \right]. \quad (29)$$

Explicit forms of the tangent, normal, and binormal vectors, along with other vectors and functions for the circular and elliptic helices are given in the appendix.

A plot of $V_c(\phi)$ for some representative values of a, b with $\omega = 4$ appears in Fig. 2. Note that the circular case values are negligible in magnitude compared to the eccentric cases, and when $a > b$, $V_c(\phi)$ is substantially larger than for the converse. For larger ratios of a to b , $V_c(\phi)$ can be orders of magnitude larger than indicated in the figure.

It is worth stating that instead of parameterizing the TH with ϕ , it would also be possible to employ an arc length scheme where an arc length parameter λ is determined from $\lambda = \int_0^\phi f(\phi') d\phi'$. However, to include the curvature potential as a function of λ , it would be necessary to find $\phi(\lambda)$ along the curve. While this could be accomplished numerically, using the azimuthal angle is somewhat better suited to incorporating external fields [29, 30].

4. Computational methods and results

If the TH is small enough to require a quantum mechanical description, the ϕ -dependent part of its wave function must obey Bloch's theorem (the t -subscript will be dropped hereafter)

$$\chi_k\left(\phi + \frac{2\pi}{\omega}\right) = \exp\left[ik\frac{2\pi}{\omega}\right]\chi_k(\phi). \quad (30)$$

A standard choice is [31]

$$\chi_k(\phi) = \exp(ik\phi)u_k(\phi) \quad (31)$$

where $u_k(\phi + 2\pi/\omega) = u_k(\phi)$ is satisfied. Single valuedness requires the Bloch index $k \equiv p = \text{integer}$. A convenient choice for $u_p(\phi)$ basis elements is

$$u_p(\beta, \phi) = \exp[i\beta\phi]. \quad (32)$$

The requirement indicated in Eq.(30) yields

$$\beta = \omega n, \quad n \equiv \text{integer}. \quad (33)$$

From the above considerations, a suitable basis set for the TH is

$$\chi^{p\alpha}(\phi) = \exp[ip\phi] \sum_n C_n^{p\alpha} \exp(in\omega\phi). \quad (34)$$

The Bloch form introduces sub-states (sub-bands in the case of a continuous rather than discrete index) for each p value which would not be present if the TH were treated as a ring of length L . The $C_m^{p\alpha}$ are the expansion coefficients for α -th sub-state of a given p value. In this work, it was found that a five-state expansion proved sufficient to yield basis size independent results for the lower p sub-states. For ω turns, values of p consistent with the Bloch theorem, $p < \omega$, are used. For clarity, only $p \geq 0$ are discussed.

A disadvantage of directly adopting the expression given by Eq.(34) is that the basis functions are not orthogonal over the integration measure $f(\phi)d\phi$. A more natural basis set is given by a re-scaled form of Eq.(34)

$$\chi^{p\alpha}(\phi) = \frac{\exp[ip\phi]}{f(\phi)^{1/2}} \sum_n C_n^{p\alpha} \exp(in\omega\phi). \quad (35)$$

With basis function orthogonality preserved on the right hand side of the Hamiltonian, eigenvalues and eigenvectors are calculated by diagonalizing the matrix comprising the elements

$$H_{mn} = \frac{1}{2\pi} \int_0^{2\pi} e^{i\omega(n-m)\phi} \left[-2V_c(\phi) - \frac{(p+\omega n)^2}{f(\phi)^2} + \frac{5}{4} \frac{f'(\phi)^2}{f(\phi)^4} - \frac{f''(\phi)}{2f(\phi)^3} \right. \\ \left. - 2i(p+\omega n) \frac{f'(\phi)}{f(\phi)^3} \right] d\phi. \quad (36)$$

Once the eigenstates are found, the current in general is calculated with (now with units)

$$\mathbf{j}(\phi, q_B, q_N) = \frac{q_e \hbar}{m_e} \text{Im} [\Psi^*(\phi, q_B, q_N) \nabla \Psi(\phi, q_B, q_N)]. \quad (37)$$

The current density given by Eq.(37) is inclusive of cross-sectional degrees of freedom and yields a current passing through a rectangular area with unit nor-

mal $\hat{\mathbf{T}}$. However, in keeping with the intent of this work, the limit of infinitesimal thickness is assumed (or equivalently, the q_B, q_N degrees of freedom are integrated out) leading to the current expression for the $p\alpha$ -th state

$$\mathbf{j}^{p\alpha}(\phi, 0, 0) = \frac{q_e \hbar}{m_e} \text{Im} \left[\frac{(\chi^{p\alpha}(\phi))^*}{f(\phi)} \frac{\partial \chi^{p\alpha}(\phi)}{\partial \phi} \right] \hat{\mathbf{T}} \quad (38)$$

where the form of the reduced gradient operator is obvious. The quantum mechanical current that stems from Eqs.(35) and (38) becomes

$$\mathbf{j}^{p\alpha}(\phi, 0, 0) = \frac{q_e \hbar}{m_e} \frac{1}{2\pi} \sum_{m,n} C_m^{p\alpha} C_n^{p\alpha} \left[\frac{(p + \omega n)}{f(\phi)^2} \cos[\omega(n-m)\phi] - \frac{f'(\phi)}{2f(\phi)^3} \sin[\omega(n-m)\phi] \right] \hat{\mathbf{T}}. \quad (39)$$

When $V_c(\phi)$ is included in the Hamiltonian the $C_m^{p\alpha}$ are modified, causing the current to become inclusive of curvature effects. This current is then used to calculate the toroidal moments according to [32]

$$\mathbf{T}_M^{p\alpha} = \frac{1}{10} \int_0^{2\pi} [(\mathbf{j}^{p\alpha}(\phi, 0, 0) \cdot \mathbf{r})\mathbf{r} - 2r^2 \mathbf{j}^{p\alpha}(\phi, 0, 0)] f(\phi) d\phi. \quad (40)$$

Equation (40) allows calculation of quantum mechanical toroidal moments of ground and excited states for each Block index p . For a macroscopic thin wire where $\mathbf{j} d\tau \rightarrow I d\mathbf{r}$ is applicable, the toroidal moment for each p reduces to the classical result

$$\mathbf{T}_M^p = \frac{I}{10} \int_0^{2\pi} \left[\left(\frac{d\mathbf{r}}{d\phi} \cdot \mathbf{r} \right) \mathbf{r} - 2r^2 \frac{d\mathbf{r}}{d\phi} \right] f(\phi) d\phi. \quad (41)$$

For circular TH, Eq.(41) yields

$$\mathbf{T}_M^p = -\frac{\pi \omega I a^2 R}{2} \hat{\mathbf{k}} \quad (42)$$

and for the elliptic TH,

$$\mathbf{T}_M^p = -\frac{\pi \omega I a b R}{2} \hat{\mathbf{k}}. \quad (43)$$

As a means of comparison, the current for the p state without curvature effects (i.e. a free particle on a given ω turn helix) is easily determined to be

$$I = \frac{2\pi q_e \hbar p}{m_e L^2} \quad (44)$$

where the total length of the TH, L , is calculated using

$$L = \int_0^{2\pi} f(\phi) d\phi.$$

The formalism described in this section was employed to calculate the eigenvalues and eigenstates expressed in terms of the $C_m^{p\alpha}$ for several ω and p values. To get a sense of the modifications arising from $V_c(\phi)$, the eigenvalues and amplitudes for a six-turn eccentric helix in a $p = 1$ state are listed without (Table 1) and with (Table 2) the curvature potential being present. The eigenvalue shifts reflect that $V_c(\phi)$ is always attractive as shown in Fig. (2), and capable of causing amplitude shifts. The reader will note there is no table indicating the shifts for the circular case; *the effects are negligible and essentially independent of the coil radius a .*

With the $C_m^{p\alpha}$ amplitudes in hand, Eq.(39) can be used to find the $\mathbf{j}^{p\alpha}(\phi, 0, 0)$ necessary for computing TMs. To set a baseline for understanding the effect of including $V_c(\phi)$, the curvature potential was shut off and $\mathbf{j}^{p\alpha}(\phi, 0, 0)$ determined for many cases. In Fig. (3), representative results are given for $\omega = 4$, $p = 1$. As anticipated, the lowest energy states yield very steady currents; oscillations begin to manifest in the higher sub-band energy states. Turning the potential on produces very little change in the currents; in Fig. (4), it becomes clear that $V_c(\phi)$ does little, which is consistent with its small amplitude indicated in Fig. (2).

When eccentricity is introduced by setting $a = .75$ and $b = .25$, the results are less trivial. The results displayed in Figs. (5) and (6) are representative of a general trend observed throughout values of ω, p . The curvature potential suppresses the current in every sub-band by a discernable fraction. Similar behavior is observed when $a = .25$ and $b = .75$ as shown in Fig. (7) and (8), but note that the magnitudes are substantially different from the converse values of a and b . The Bloch form of the wave function, independent of the presence of $V_c(\phi)$ (which again lessens the magnitude of the currents), the Bloch form of the wave function and the ab dependence of the Laplacian are sufficient to cause asymmetries in the currents.

Toroidal moment results for $\omega = 4$ are shown in Table 3 for several p -states and their corresponding sub-states. For a given p value, the lowest energy state in Table 3 agrees very well with the value obtained if the current given by Eq.(44) were used, although $V_c(\phi)$ can shift the ordering of states in a way to reorder the ground state moment as seen for the $p = 3$ states. In isolation, this is relatively unimportant. However, in a broader context where the natural temperature scale of a 1000\AA helix is a few μK , thermodynamic averages of the type

$$\langle T_M \rangle = \sum T_M(E_n) \exp[-E_n/\tau] \quad (45)$$

will necessitate accounting for proper ordering.

The modifications to the TMs for the upright ($b > a$) coil situation are generally minimal with exceptions only for $p = 2$. The flattened coil ($a > b$) results in Table 3 show a much stronger variation in TM values, consistent with the much larger strength of $V_c(\phi)$ for $a > b$ relative to the converse. A sense of the dependence of TMs on ω can be gleaned from Table 4 where now $\omega = 8$. Increased variation is seen for both eccentricities, but the flattened coil case demonstrates appreciable deviation from the classical expression.

5. Conclusions

In this work a prescription to include curvature at the nanoscale for particles constrained to toroidal helices was presented, which the authors applied toward a quantum mechanical calculation of toroidal moments. It is worth emphasizing that the curvature inclusive reduced dimensionality Schrödinger equation developed here is driven by an interest in having more tractable, effective models for nanomaterials, and is done with the aim of eventually confronting experimental data rather than as a purely theoretical exercise. In that context, the choice to consider helices was driven by their capability of producing toroidal moments, which are currently of both theoretical and practical interest. The curvature potential for the helix was derived and shown to be the dominant part of the Hamiltonian for lower energy eigenstates of eccentric helices. An intriguing

result that arose here was a demonstrated *ab* asymmetry in several states of the quantum mechanically calculated $\mathbf{T}_M^{p\alpha}$, an asymmetry not exhibited in the classical expression of Eq.(43).

The array of results given in this work was limited to relatively small values of ω and to less severe eccentricity because of numerical limitations on evaluating integrals of the type shown in Eq.(36). The extension to larger values of ω were considered (at least currently) outside the scope of what the authors were attempting to accomplish. However, preliminary work gives some indication that *Mathematica* is capable of performing the necessary integrals, albeit with increased time expense. It would be of interest to investigate more extreme cases of eccentricity and loop number given the enhancement of moments already evidenced by larger ω .

Tailoring the response of toroidal helices to electromagnetic radiation by fabricating objects with curvature as a free parameter is still well outside the reach of current fabrication methods. However, the formalism and basis set established here may serve as means for further investigation of the $\mathbf{T}_M \cdot \partial \mathbf{E} / \partial t$ interactions relevant to the coupling of toroidal moments to electromagnetic fields. The extension of the methods here to cases where external vector potentials are present may be naturally developed from work already done for tori immersed in arbitrary magnetic fields [29] and is ongoing with an aim to understanding persistent current effects.

Finally, debate as to whether curvature effects are relevant to, and how they are manifested in, topologically novel nanostructures may eventually be settled by examining systems akin to toroidal helices. By opting to either include or exclude curvature potentials in modeling routines, it may prove true that sensitive quantities like toroidal moments will provide a clear signature as to the influence of V_c . Work such as that done in this paper may hopefully contribute to a resolution to the question of how to properly incorporate twists and turns in the quantum mechanical description of bent nanostructures.

Appendix

This appendix presents a more complete set of formulae for the circular TH as well as a corresponding set for the elliptical case.

A.1 The circular case

$$\hat{\boldsymbol{\theta}} = -\sin(\omega\phi)\hat{\boldsymbol{\rho}} + \cos(\omega\phi)\hat{\mathbf{k}} \quad (\text{A-1})$$

$$\hat{\mathbf{n}} = \cos(\omega\phi)\hat{\boldsymbol{\rho}} + \sin(\omega\phi)\hat{\mathbf{k}} \quad (\text{A-2})$$

$$f(\phi) = (a^2\omega^2 + W(\phi)^2)^{1/2} \quad (\text{A-3})$$

$$\hat{\mathbf{e}}_2 = \frac{W(\phi)\hat{\boldsymbol{\theta}} - a\omega\hat{\boldsymbol{\phi}}}{f(\phi)} \quad (\text{A-4})$$

$$P_1(\phi) = -\frac{a\omega^2 + W(\phi)\cos(\omega\phi)}{f(\phi)^2} \quad (\text{A-5})$$

$$P_2(\phi) = \frac{\sin(\omega\phi)}{f(\phi)} \left[1 + \left(\frac{a\omega}{f(\phi)} \right)^2 \right] \quad (\text{A-6})$$

$$\kappa(\phi) = (P_1^2(\phi) + P_2^2(\phi))^{1/2} \quad (\text{A-7})$$

$$\hat{\mathbf{T}} = \frac{a\omega\hat{\boldsymbol{\theta}} + W(\phi)\hat{\boldsymbol{\phi}}}{f(\phi)} \quad (\text{A-8})$$

$$\hat{\mathbf{N}} = \frac{1}{\kappa(\phi)}(P_2(\phi)\hat{\mathbf{e}}_2 + P_1(\phi)\hat{\mathbf{n}}) \quad (\text{A-9})$$

$$\hat{\mathbf{B}} = \frac{1}{\kappa(\phi)}(-P_1(\phi)\hat{\mathbf{e}}_2 + P_2(\phi)\hat{\mathbf{n}}) \quad (\text{A-10})$$

A.2 The elliptic case

With $W(\phi) = R + a \cos(\omega\phi)$, the equation of the elliptic toroidal helix is

$$\mathbf{r}(\phi) = W(\phi)\hat{\boldsymbol{\rho}} + b \sin(\omega\phi)\hat{\mathbf{k}}.$$

The extension of the results of Sec. A.1 to the elliptic case is straightforward:

$$P(\phi) = [a^2 \sin^2(\omega\phi) + b^2 \cos^2(\omega\phi)]^{1/2} \quad (\text{A-11})$$

$$\hat{\boldsymbol{\theta}}_E = \frac{1}{P(\phi)}[-a \sin(\omega\phi)\hat{\boldsymbol{\rho}} + b \cos(\omega\phi)\hat{\mathbf{k}}] \quad (\text{A-12})$$

$$\hat{\mathbf{n}}_E = \frac{1}{P(\phi)} [b \cos(\omega\phi) \hat{\boldsymbol{\rho}} + a \sin(\omega\phi) \hat{\mathbf{k}}] \quad (\text{A-13})$$

$$\hat{\mathbf{e}}_2 = \frac{W(\phi) \hat{\boldsymbol{\theta}}_E + P(\phi) \omega \hat{\boldsymbol{\phi}}}{f(\phi)} \quad (\text{A-14})$$

$$f(\phi) = (P(\phi)^2 \omega^2 + W(\phi)^2)^{1/2} \quad (\text{A-15})$$

$$P_1(\phi) = -\frac{b}{P(\phi)} \frac{a\omega^2 + W(\phi) \cos(\omega\phi)}{f(\phi)^2} \quad (\text{A-16})$$

$$P_2(\phi) = \frac{\sin(\omega\phi)}{f(\phi)} \left(\frac{a}{P(\phi)} + \frac{\omega^2 W(\phi) (a^2 - b^2) \cos(\omega\phi) + P(\phi)^2 a \omega^2}{f(\phi)^2 P(\phi)} \right) \quad (\text{A-17})$$

$$\kappa(\phi) = (P_1(\phi)^2 + P_2(\phi)^2)^{1/2} \quad (\text{A-18})$$

$$\hat{\mathbf{T}} = \frac{P(\phi) \omega \hat{\boldsymbol{\theta}}_E + W(\phi) \hat{\boldsymbol{\phi}}}{f(\phi)} \quad (\text{A-19})$$

$$\hat{\mathbf{N}} = \frac{1}{\kappa(\phi)} (P_2(\phi) \hat{\mathbf{e}}_2 + P_1(\phi) \hat{\mathbf{n}}_E) \quad (\text{A-20})$$

$$\hat{\mathbf{B}} = \frac{1}{\kappa(\phi)} (-P_1(\phi) \hat{\mathbf{e}}_2 + P_2(\phi) \hat{\mathbf{n}}_E) \quad (\text{A-21})$$

References

- [1] M. Wegener, S. Linden, *Physics Today* 63 (2010) 32.
- [2] H. Zhang, S. W. Chung, C. A. Mirkin, *Nano. Lett.* 3 (2003) 43.
- [3] H.R.Shea, R. Martel, P. Avouris, *Phys. Rev. Lett.* 84 (2000) 4441.
- [4] A. Lorke, R. J. Luyken, A. O. Govorov, J. P. Kotthaus, *Phys. Rev. Lett.* 84 (2000) 2223.
- [5] A. Chaplik, R. H. Blick, *New J. Phys.* 6 (2004) 33.
- [6] R. C. T. da Costa, *Phys. Rev. A* 23 (1981) 1982.
- [7] R. C. T. da Costa, *Phys. Rev. A* 25 (1982) 2893.
- [8] P. Duclos, P. Exner, *Rev. Math. Phys.* 7 (1995) 73.
- [9] M. Encinosa, B. Etemadi, *PRA* 58 (1998) 77.
- [10] M. Encinosa, B. Etemadi, *Physica B* 266 (1998) 361.
- [11] B. Jensen, H. Koppe, *Ann. of Phys.* 63 (1971) 586.
- [12] S. Matusani, *J. Phys. Soc. Jap.* 61 (1991) 55.
- [13] S. Matsutani, *Rev. Math. Phys.* 11 (1999) 171.
- [14] H. Taira, H. Shima, *Surf. Sci.* 601 (2007) 5270.
- [15] T. Kaelberer, V. Fedetov, N. Papasimakis, D. Tsai, N. Zheludev, *Science* 330 (2010) 1510.
- [16] G. F. Afanasiev, V. M. Dubovik, G. Goldoni, F. Troiani, E. Molinari, *Phys. Part. Nucl.* 29 (1998) 366.
- [17] A. Ceulemans, L. Chibotaru, P. Fowler, *Phys. Rev. Lett.* 80 (1998) 1861.
- [18] V. M. Dubovik, V. V. Tugushev, *Phys. Rep.* 187 (1990) 145.

- [19] N. Papasimakis, V. A. Fedotov, K. Marinov, N. I. Zheludev, Phys. Rev. Lett. 103 (2009) 093901.
- [20] I. Naumov, L. Bellaiche, H. Fu, Nature 432 (2004) 737.
- [21] N. A. Spaldin, M. Fiebig, M. Mostovoy, J. Phys.: Condens. Matter 20 (2008) 1.
- [22] K. Sawada, N. Nagaosa, Phys. Rev. Lett. 95 (2005) 237402.
- [23] O. Kibis, M. Portnoi, Tech. Phys. Lett. 33 (2007) 878.
- [24] P. C. Schuster, R. L. Jaffe, Ann. Phys. 307 (2003) 132.
- [25] M. Burgess, B. Jensen, Phys. Rev. A 48 (1993) 1861.
- [26] M. Encinosa, L. Mott, B. Etemadi, Phys. Scr. 72 (2005) 13.
- [27] W. C. Graustein, Differential Geometry, 2nd Edition, Dover, New York, 1962.
- [28] G. Arfken, H. Weber, Mathematical Methods for Physicists, 6th Edition, Elsevier Academic Press, Burlington MA, 2002.
- [29] M. Encinosa, Physica E 28 (2005) 209.
- [30] M. Encinosa, J. Comput. Aided Mater. Des. 14 (2006) 65.
- [31] G. Grosso, G. P. Parravicini, Solid State Physics, 1st Edition, Academic Press, SanDiego, 2002.
- [32] K. Marinov, A. D. Boardman, V. A. Fedotov, N. Zheludev2, N. J. Phys. 9 (2007) 324.

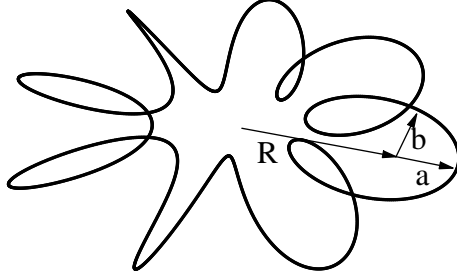


Fig. 1: A toroidal helix where R is the distance from the center of the TH to a center of a loop of the TH. The parameter a is the TH's maximum perpendicular horizontal distance from a concentric cylinder of radius R . The parameter b is the TH's maximum vertical distance from the x-y plane.

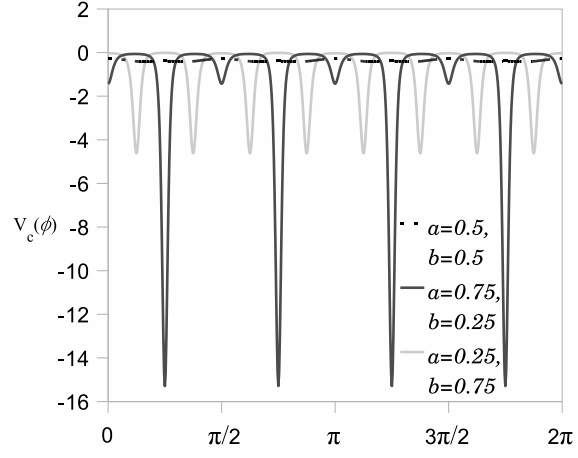


Fig. 2: The curvature potential $V_c(\phi)$ in units of $\hbar^2/(m_e R^2)$ for the case of the circular TH with $R = 1$, $\omega = 4$, $a = b = 0.5$ and two elliptic TH cases: $R = 1$, $\omega = 4$, $a = 0.25$, $b = 0.75$ and $R = 1$, $\omega = 4$, $a = 0.25$, $b = 0.75$.

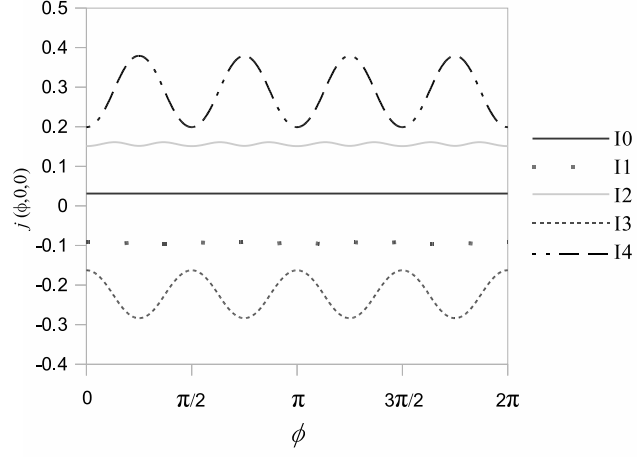


Fig. 3: $j^{p\alpha}(\phi, 0, 0) \equiv I(\phi)$ in units of $q_e \hbar / (m_e R^2)$ for five eigenstates of the circular TH configuration $\omega = 4$, $a = 0.5$, $b = 0.5$, $R = 1$, $p = 1$ where $V_c(\phi)$ is neglected.

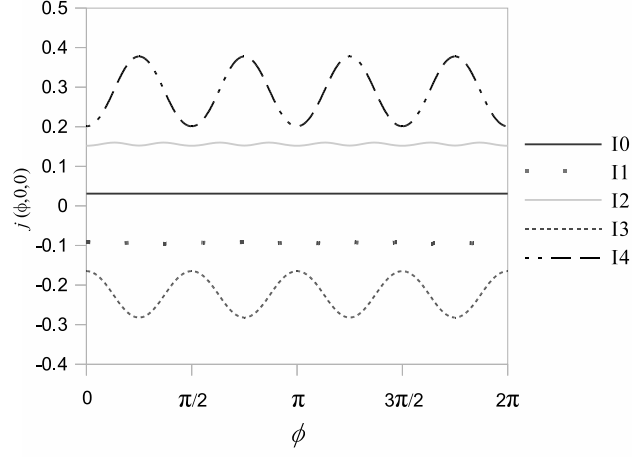


Fig. 4: $j^{p\alpha}(\phi, 0, 0) \equiv I(\phi)$ in units of $q_e \hbar / (m_e R^2)$ for five eigenstates of the circular TH configuration $\omega = 4$, $a = 0.5$, $b = 0.5$, $R = 1$, $p = 1$ with $V_c(\phi)$. Curvature effects on the current are small in the circular case.

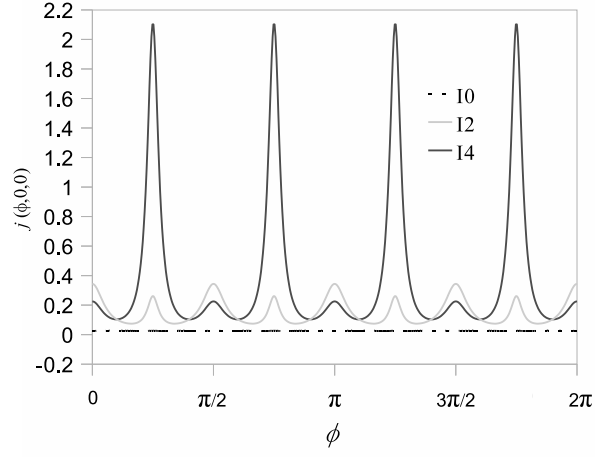


Fig. 5: $j^{p\alpha}(\phi, 0, 0) \equiv I(\phi)$ corresponding to the ground state, and second and fourth excited states in units of $q_e \hbar / (m_e R^2)$, for the elliptic TH configuration $\omega = 4$, $a = 0.75$, $b = 0.25$, $R = 1$, $p = 1$, without the curvature potential $V_c(\phi)$.

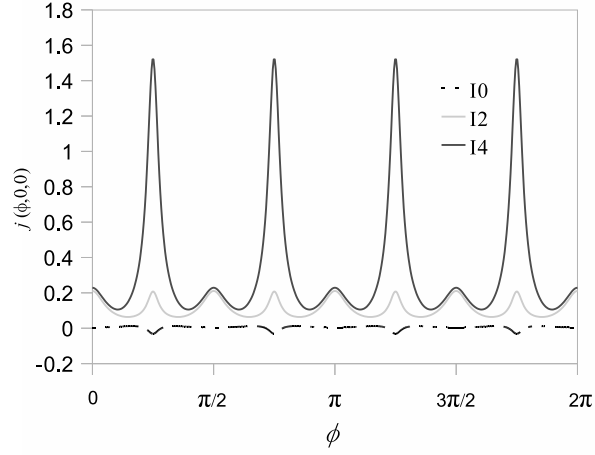


Fig. 6: $j^{p\alpha}(\phi, 0, 0) \equiv I(\phi)$ corresponding to the ground state, and second and fourth excited states in units of $q_e\hbar/(m_e R^2)$, for the elliptic TH configuration $\omega = 4$, $a = 0.75$, $b = 0.25$, $R = 1$, $p = 1$ inclusive of the curvature potential $V_c(\phi)$. Inclusion of the curvature potential causes a reduction in amplitude for each j .

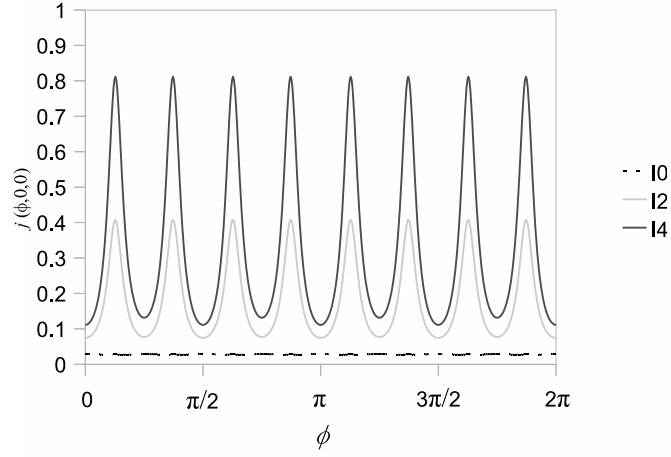


Fig. 7: $j^{p\alpha}(\phi, 0, 0) \equiv I(\phi)$ corresponding to the ground state, and second and fourth excited states in units of $q_e \hbar / (m_e R^2)$ for the elliptic TH configuration $\omega = 4$, $a = 0.25$, $b = 0.75$, $R = 1$, $p = 1$ without curvature potential.

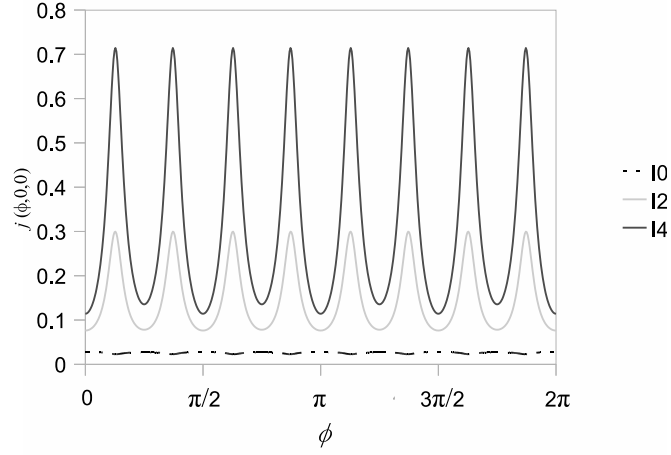


Fig. 8: $j^{p\alpha}(\phi, 0, 0) \equiv I(\phi)$ corresponding to the ground state, and second and fourth excited states in units of $q_e \hbar / (m_e R^2)$ for the configuration $\omega = 4$, $a = 0.25$, $b = 0.75$, $R = 1$, $p = 1$ inclusive of the curvature potential. When the curvature potential is included in the calculation of $I(\phi)$, the current is reduced in amplitude.

	E_0	E_1	E_2	E_3	E_4
	0.0724	1.6369	3.0045	7.7907	10.9186
m	$C_m^{(0)}$	$C_m^{(1)}$	$C_m^{(2)}$	$C_m^{(3)}$	$C_m^{(4)}$
-2	-0.1055	-0.1648	-0.0607	-0.9761	0.0722
-1	0.0585	-0.9762	-0.1236	0.1631	-0.0428
0	0.9822	0.0315	0.0291	-0.1020	0.1520
1	0.0556	0.1374	-0.9702	0.0171	-0.1907
2	-0.1331	-0.0087	-0.1970	0.0996	0.9662

Table 1: Eigenvalues and amplitudes $C_m^{(\alpha)}$ for an $\omega=6$, $a=0.75$, $b=0.25$, $R=1$, $p=1$ elliptic TH neglecting curvature effects.

	E_0	E_1	E_2	E_3	E_4
	-1.4739	-0.0442	2.1393	5.7258	9.2713
m	$C_m^{(0)}$	$C_m^{(1)}$	$C_m^{(2)}$	$C_m^{(3)}$	$C_m^{(4)}$
-2	0.0606	-0.0310	0.1231	-0.9410	0.3077
-1	-0.3794	-0.7975	0.4620	0.0389	-0.0713
0	0.8927	-0.4441	-0.0424	0.0579	-0.0266
1	-0.2353	-0.4071	-0.8712	-0.0772	0.1179
2	-0.0062	0.0118	-0.1027	-0.3220	-0.9411

Table 2: Eigenvalues and amplitudes $C_m^{(\alpha)}$ for an $\omega=6$, $a=0.75$, $b=0.25$, $R=1$, $p=1$ elliptic TH including curvature effects.

Table 3: Toroidal moments for two configurations with $\omega=4$. TM's with and without curvature effects, and classical calculation for each case.

ω	a	b		
4	0.25	0.75		
p	TM	TM w/ $V_c(\phi)$	ratio	Classical TM
1	-0.0334	-0.0317	1.0545	-0.0332
1	0.0895	0.0718	1.2457	
1	-0.1478	-0.1308	1.1293	
1	0.1901	0.1837	1.0347	
1	-0.2401	-0.2347	1.0230	
2	-0.0669	-0.0551	1.2129	-0.0664
2	0.0600	0.0524	1.1452	
2	-0.0088	0.0193	-0.4562	
2	-0.0031	-0.0344	0.0896	
2	-0.2646	-0.2655	0.9967	
3	0.0288	0.0305	0.9430	-0.0995
3	-0.0993	-0.0798	1.2441	
3	0.1380	0.1203	1.1479	
3	-0.2038	-0.2052	0.9930	
3	-0.2888	-0.2908	0.9931	

ω	a	b		
4	0.75	0.25		
p	TM	TM w/ $V_c(\phi)$	ratio	Classical TM
1	-0.0317	-0.0068	4.6359	-0.0319
1	0.1625	0.0627	2.5936	
1	-0.2697	-0.1743	1.5468	
1	0.1505	0.1470	1.0240	
1	-0.1694	-0.1863	0.9096	
2	-0.0561	0.0000	-	-0.0638
2	0.1067	0.0157	6.7927	
2	-0.3206	-0.1161	2.7623	
2	0.1298	-0.0081	-15.9737	
2	-0.1755	-0.2072	0.8472	
3	0.0664	0.0063	10.5665	-0.0957
3	-0.0933	-0.0346	2.6957	
3	0.1211	0.1092	1.1090	
3	-0.3893	-0.3413	1.1407	
3	-0.1784	-0.2131	0.8372	

Table 4: Toroidal moments for two configurations with $\omega=8$. TM's with and without curvature effects, and classical calculation for each case.

ω	a	b		
8	0.25	0.75		
p	TM	TM w/ $V_c(\phi)$	ratio	Classical TM
1	-0.0190	-0.0166	1.1485	-0.0195
1	0.1218	0.0441	2.7619	
1	-0.1600	-0.0822	1.9477	
1	0.2787	0.1938	1.4383	
1	-0.3175	-0.2351	1.3501	
2	-0.0386	-0.0332	1.1615	-0.0390
2	0.1123	0.0664	1.6917	
2	-0.1890	-0.1430	1.3217	
2	0.2635	0.2293	1.1490	
2	-0.3401	-0.3113	1.0923	
3	-0.0582	-0.0490	1.1888	-0.0584
3	0.0952	0.0699	1.3622	
3	-0.2104	-0.1853	1.1354	
3	0.2454	0.2238	1.0966	
3	-0.3598	-0.3472	1.0363	

ω	a	b		
8	0.75	0.25		
p	TM	TM w/ $V_c(\phi)$	ratio	Classical TM
1	-0.0189	-0.0096	1.9789	-0.0192
1	0.2454	0.0560	4.3789	
1	-0.3224	-0.1299	2.4826	
1	0.3520	0.2586	1.3612	
1	-0.3971	-0.3162	1.2558	
2	-0.0378	-0.0157	2.4149	-0.0383
2	0.2267	0.0757	2.9954	
2	-0.3806	-0.2231	1.7056	
2	0.3382	0.2988	1.1315	
2	-0.4284	-0.4176	1.0257	
3	-0.0565	-0.0138	4.1053	-0.0575
3	0.1951	0.0614	3.1800	
3	-0.4221	-0.2692	1.5680	
3	0.3116	0.2627	1.1858	
3	-0.4509	-0.4640	0.9718	